

A New Heptadentate Picolinate–Based Ligand and Its Corresponding Gd(III) Complex: the Effect of Picolinate *versus* Acetate Pendant on Complex Property

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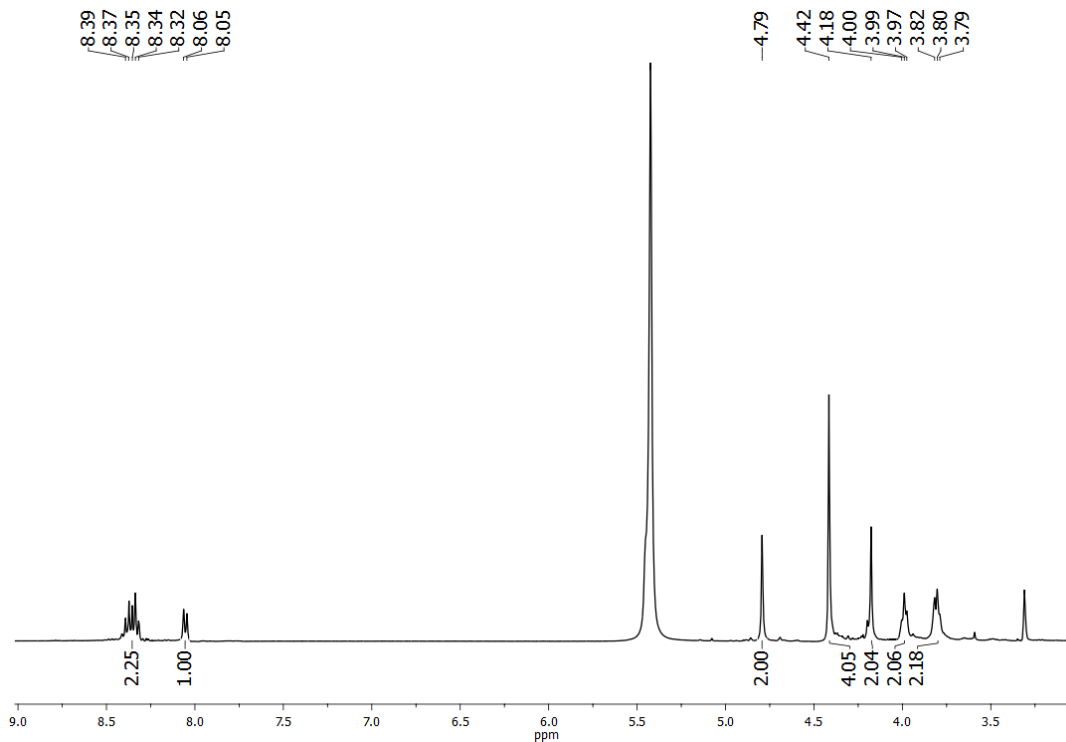


Figure S1. ^1H NMR spectrum of H_4peada measured in CD_3OD solvent.

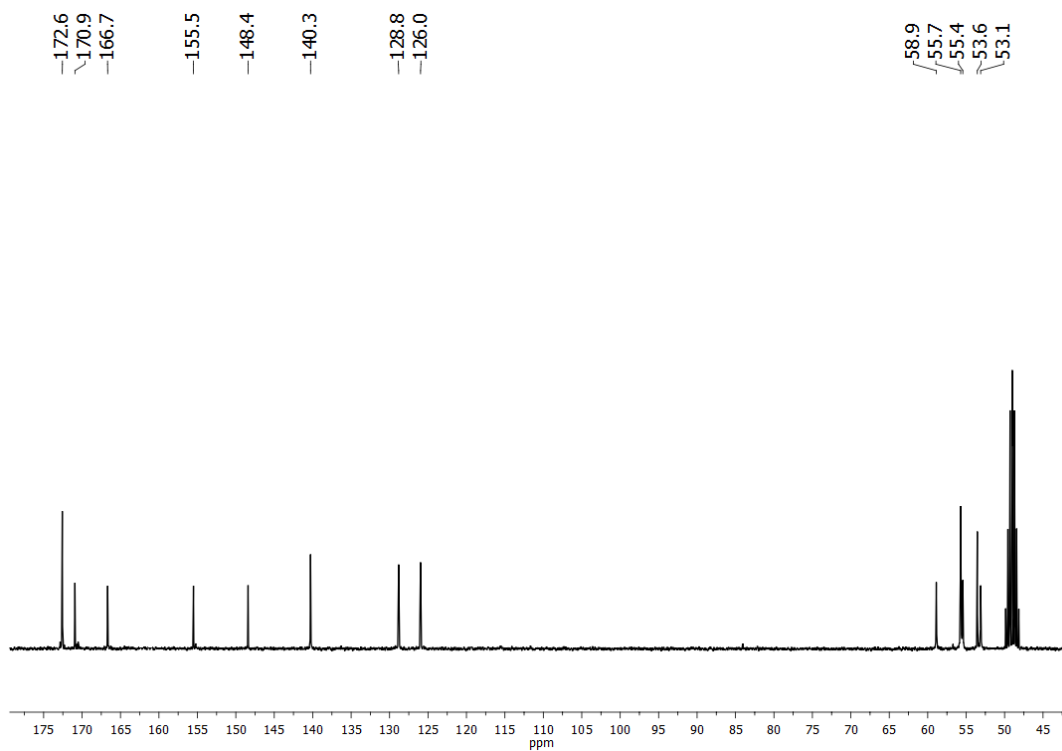


Figure S2. ^{13}C NMR spectrum of ligand H_4peada measured in CD_3OD solvent.

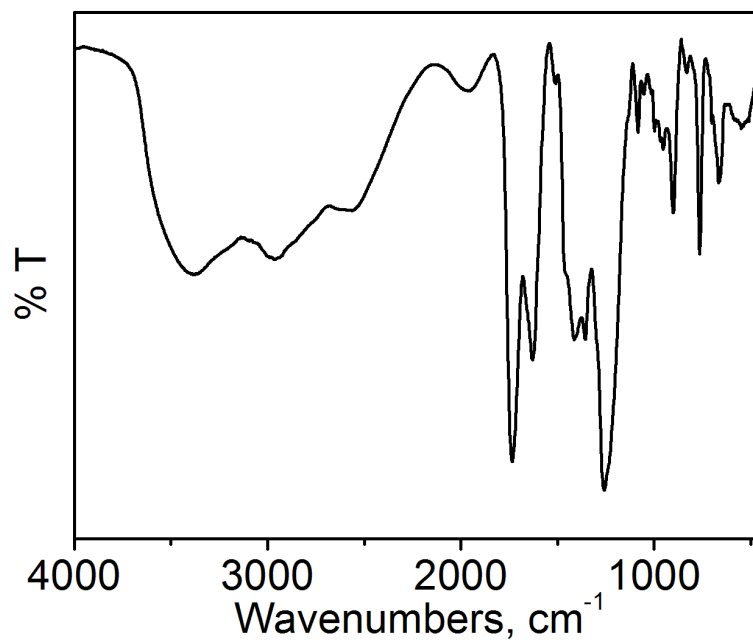


Figure S3. FTIR spectrum of ligand H₄peada.

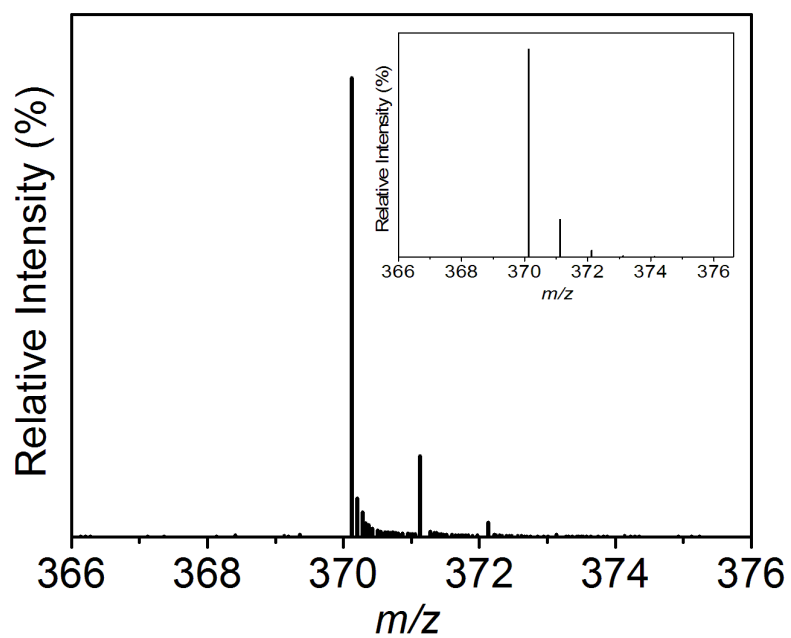


Figure S4. ESI-MS (+ve) mass spectrum of ligand H₄peada. Simulated spectrum has been given as inset.

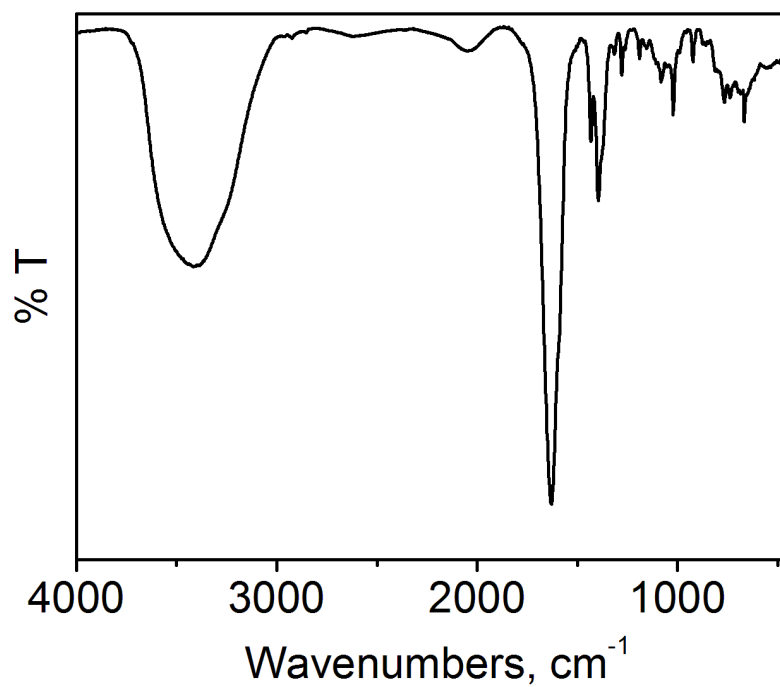


Figure S5. FTIR spectrum of complex **1**.

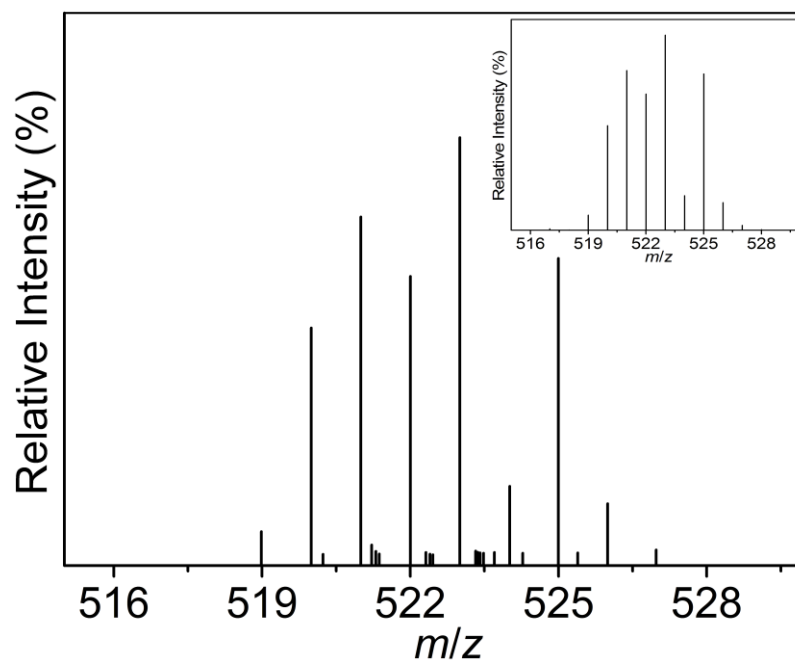


Figure S6. ESI-MS (-ve) mass spectrum of complex **1**. Simulated spectrum has been given as inset.

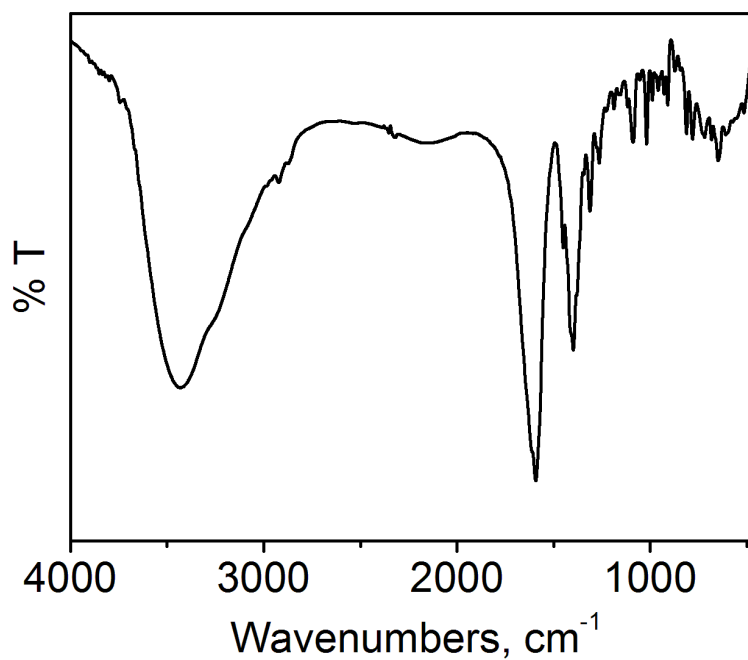


Figure S7. FTIR spectrum of complex 2.

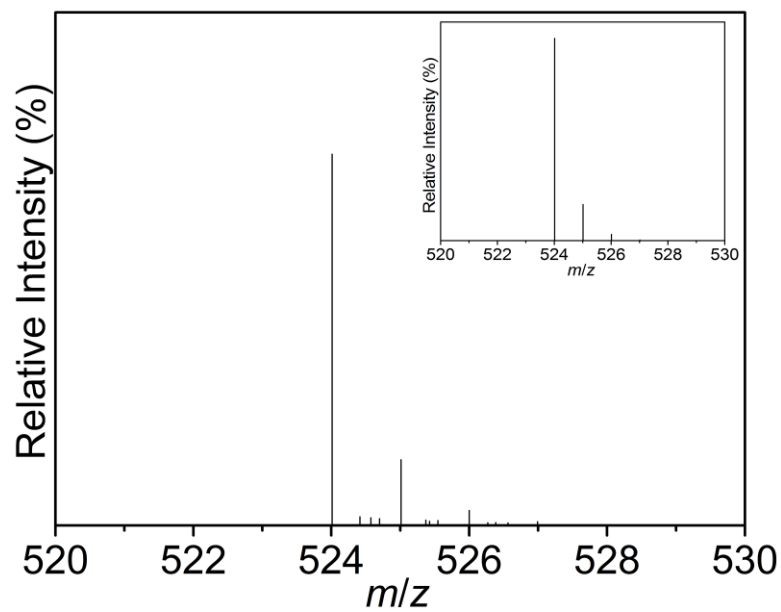


Figure S8. ESI-MS (-ve) mass spectrum of complex 2. Simulated spectrum has been given as inset.

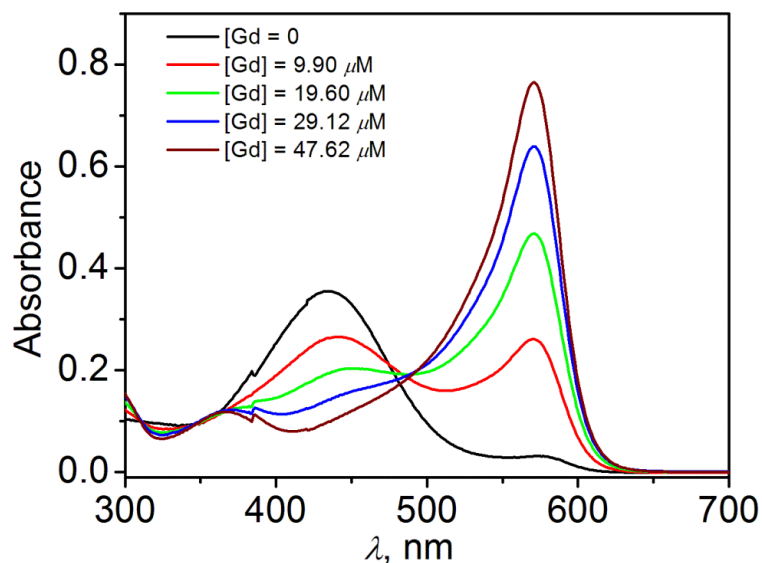


Figure S9. UV-vis spectrum of xylenol orange solution in acetate buffer (pH = 5.8) in the presence of varied concentrations of Gd(III) ions, from zero to 47.62 μM .

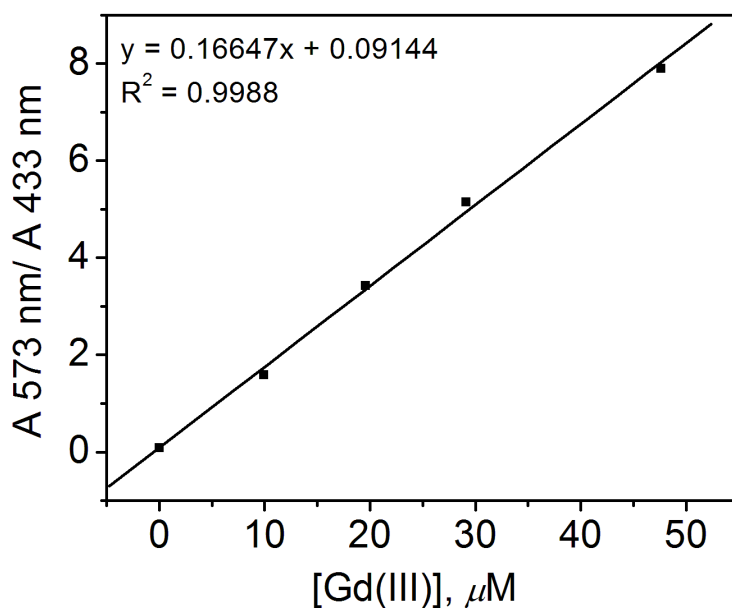


Figure S10. Calibration curve obtained from the spectrophotometric changes of xylenol orange (in acetate buffer, pH = 5.8) absorptions in the presence of varied concentrations of Gd(III) ions. For 50 μL of complex **1** ([complex **1**] = 27.5 mM) in 2.0 mL xylenol orange solution (pH = 5.8), $A_{573\text{ nm}}/A_{433\text{ nm}} = 0.0987$.